2-amino-3-(4-chlorophenyl)sulfonylpropanoic acid 5445-04-5 | DTXSID30396827

0440 04 0	DINOIDC	70030027	

Model Performance

Model	Data
IVIOGCI	Data

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.85	0.69	0.86	0.67	0.86	0.78	

Model Results

Predicted value: 8.76e-01

Global applicability domain: Inside

Local applicability domain index: 5.39e-01

Confidence level: 7.71e-01

Nearest Neighbors from the Training Set

Image not found

CHEMBL106848 Measured: 0.36 Predicted: 8.41e-01

Image not found

3-Fluoro-4-[(2-

hydroxyethyl)sulfanyl]benzene-1-

sulfonamide Measured: 0.72 Predicted: 8.92e-01